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HIGH PRODUCTION VOLUME (HPV)

CHALLENGE PROGRAM

FINAL SUBMISSION

For

Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental and Regulatory Task Group

December 2006

LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP

The Health, Environmental and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

Afton Corporation (formerly Ethyl Corporation)

Chevron Oronite Company, LLC

Infineum

The Lubrizol Corporation

EXECUTIVE SUMMARY

The Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council submits this final submission for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide (CAS numbers 18760-44-6 or 398141-87-2) to the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program.

Fate and Transport Characteristics. Based on the physicochemical properties and molecular structure, thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is most likely to partition to soils and water. The HERTG calculated fugacity data on thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. Since this material lacks any readily hydrolyzable moieties, hydrolysis modeling was not conducted. . Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide was subjected to biodegradability testing and found to be poorly biodegradable. The HERTG developed computer modeled data that indicated thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide does not possess the potential to photodegrade.

Aquatic Toxicology. Data on algal toxicity was reviewed and additional aquatic toxicity studies were completed. The findings of the completed tests and available studies indicated thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is toxic to fish, aquatic invertebrates, and algae.

Mammalian Toxicology - Acute. Data on acute mammalian toxicity (oral and dermal) were reviewed. Oral and dermal LD_{50} levels for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide were very high, indicating essentially no toxicity.

Mammalian Toxicology - Subchronic Toxicity. The HERTG reviewed a repeated-dose study for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. After administration of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide to rats, the liver and kidneys were mildly affected. However, since the effects were both mild and observed primarily at high doses, the results indicate that thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide possesses a low order of repeated-dose toxicity to mammals.

Mammalian Toxicology - Reproductive and Developmental Toxicity. The HERTG investigated the reproductive and developmental toxicity of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. Administration of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide did not impact fertility or reproduction in rats. Additionally, this material did not cause any developmental effects in offspring, thus indicating thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide does not cause reproductive or developmental toxicity.

Mammalian Toxicology - Mutagenicity. Data from a bacterial reverse mutation assay was available for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide and the results were negative for mutagenicity, both with and without metabolic activation. Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide was also tested in an *in vitro* chromosomal aberration assay. The results were negative for clastogenicity, both with and without metabolic activation.

Conclusion. Based on the available data and physiochemical, environmental fate, aquatic toxicity and mammalian toxicity studies completed for this submission, the HERTG concluded that thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is toxic to aquatic organisms but the overall risk is low to

mammals. As this final submission was completed, the HERTG carefully evaluated the number of animals necessary for testing and the conditions to which animals might be exposed. Thus, a minimal amount of testing involving the use of animals was employed.

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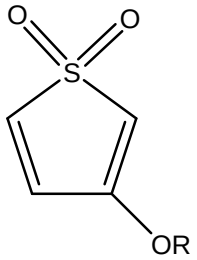
1.0 INTRODUCTION

In March 1999, the Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council (ACC) committed to address data needs for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This final submission follows up on that commitment. Specifically, this final submission sets forth how the HERTG fulfilled the Screening Information Data Sets (SIDS) requirements for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide (CAS Numbers: 18760-44-6 or 398141-87-2; representative structure shown in Figure 1). Note, a voluntary CAS number correction for CAS # 18760-44-6 was submitted to the EPA and as result, CAS # 398141-87-2 was established as the updated CAS number. Therefore, CAS #s 398141-87-2 and 18760-44-6 refer to the same material in this final submission.

FIGURE 1. CHEMICAL STRUCTURE OF THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE



R= $C_{9\text{-}11}$ –isoalkyl, C_{10} rich
Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide
CAS No.: 18760-44-6 or 398141-87-2
Molecular Weight: 276.4 grams/mole

In preparing this final submission, the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physiochemical properties, mammalian toxicity endpoints, and environmental fate and effects for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physiochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation. Where additional data was needed, testing was completed to meet the SIDS requirements.

2.0 USE AND EXPOSURE INFORMATION

The substance, thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, is a lubricating additive in many types of internal combustion engine oils, automatic transmission fluids, and hydraulic fluids.

Based on the uses, the potentially exposed populations include (1) workers involved in the manufacture of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, blending this component into additive packages, and blending the additive packages into finished lubricants; (2) quality assurance workers who sample and analyze these products to ensure that they meet specifications; (3) workers involved in the transfer and transport of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, additive packages or finished lubricants that contain this component; (4) mechanics who may come into contact with both fresh and used lubricants while working on engines or equipment; (5) service station attendants and consumers who may periodically add lubricating oil to automotive crankcases; and (6) consumers who may change their own automotive engine oil. The most likely route of human exposure for these substances is through dermal contact. The most likely source of environmental exposure is accidental spills at manufacturing sites or during transport.

3.0 PHYSIOCHEMICAL PROPERTIES

The physiochemical properties of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide are shown in table 1, below.

TABLE 1. PHYSIOCHEMICAL PROPERTIES OF THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE

Physical/Chemical Characteristics	Study Results
Melting Point	Not Applicable
Boiling Point	360^{o} C [1]
Vapor Pressure	8.62 x 10^{-6} mm Hg @ 25^{o} C [1]
Partition Coefficient	1.19 (OECD 117 method)
Water Solubility	54 mg/L at 20^{o}C (EEC Commission Directive 92/69/EEC Method A6 Water Solubility)

[1] Modeled value using EpiWin version 3.12 software

4.0 ENVIRONMENTAL FATE DATA

4.1 Biodegradability

A modified Sturm test (OECD Guideline 301B) was available to evaluate the biodegradability of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. After 28 days, the extent of biodegradation was 9.6% based on total carbon dioxide production. This available data were considered adequate and reliable.

4.2 Hydrolysis

There are no published or unpublished hydrolysis studies on thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. However, thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide does not contain any readily hydrolyzable moieties and as a result, this material is unlikely to undergo hydrolysis. Therefore, hydrolysis modeling was not conducted.

4.3 Photodegradation

There are no published or unpublished photodegradation studies of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. The Atmospheric Oxidation Potential (AOP) of this substance was characterized using the modeling program AOPWIN. The results indicated this material has a low potential for photodegradation (Table 2)

4.4 Fugacity Modeling

There are no published or unpublished fugacity data for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. The relative distribution among environmental compartments was estimated using Level III Fugacity modeling. The modeling indicated this material will primarily partition to water and soils.

TABLE 2. ENVIRONMENTAL FATE DATA FOR THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE

Environmental Fate	Study Results
Biodegradation	9.6% at 28 days (OECD 301B)
Photodegradation[1]	AOPWIN Model Estimation OH- Rate Constant (cm3/molec-sec) = 274.6 x 10^{-12} Half-life = 0.039 days
Fugacity[1]	Mass distribution (%) Air 0.163 Water 43.2 Soil 56.5 Sediment 0.0907

[1] Modeled values using EpiWin version 3.12 and measured water solubility value of 54 mg/L and log K_{ow} value of 1.19.

5.0 ECOTOXICOLOGY DATA

5.1 Fish Acute Toxicity

An acute fish toxicity study was conducted for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide and the 96 hour LC_{50} of for rainbow trout (*Pimephales promelas*) was 4.2 mg/L and the no observed effect concentration (NOEC) was 1.5 mg/L.

5.2 Acute Invertebrate Toxicity

Acute invertebrate toxicity study was conducted for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide and the 48 hour EC_{50} for *Daphnia magna* was 2.5 mg/L and the no observed effect concentration (NOEC) was 0.63 mg/L.

5.3 Algal Toxicity

An adequate and reliable algal tox study was available and the 96 hour EL_{50} of freshwater algae (*Scenedesmus subspicatus*) exposed to thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide was 3.5 mg/L WAF and the NOEL was 0.313 mg/L.

TABLE 3. AQUATIC TOXICITY DATA FOR THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE (CAS #S 18760-44-3 OR 398141-87-2)

Ecotoxicity study	Study Results
Acute Toxicity to Fish (OECD 203) (*Pimephales promelas*)	96-hour LC_{50} = 4.2 mg/L WAF NOEC = 1.5 mg/L WAF
Acute Toxicity to Invertebrates (OECD 202) (*Daphnia magna*)	48-hour EC50 = 2.5 mg/L WAF NOEC = 0.63 mg/L WAF
Acute Toxicity to Algae (OECD 201) (*Scenedesmus subspicatus*)	EL_{50} (72 hrs) = 3.5 mg/L WAF NOEL = 0.313 mg/L WAF

WAF: Water accommodated fraction

6.0 MAMMALIAN TOXICOLOGY DATA

6.1 Acute Mammalian Toxicity

Acute oral and dermal toxicity studies were available for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. The LD_{50} in rats (oral) and rabbits (dermal) were >10 g/kg and between 4 and 8 g/kg, respectively.

6.2 Repeated-dose Toxicity

A repeat dose toxicity study for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide was available. Although the liver and kidneys of males and females were mildly affected primarily with administration of the two highest doses (500 and 1000 mg/kg/day), this material did not cause significant toxicity to rats (Table 4.)

6.3 Reproductive and Developmental Toxicity

The HERTG conducted a reproductive and developmental screening study (OECD 421) in rats on thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. Administration of this material did not impact fertility or reproduction and did not cause developmental toxicity (Table 4).

TABLE 4. MAMMALIAN TOXICITY DATA FOR THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE (CAS #S 18760-44-3 OR 398141-87-2)

Mammalian Toxicity	Study Results
Acute Toxicity	Rat Oral LD_{50} >10 g/kg Rabbit Dermal LD_{50} between 4 and 8 g/kg
Repeat Dose Toxicity	Oral gavage 28-day study in rats (OECD 407) Female NOEL = 100 mg/kg/day Male NOEL = not identified because of presence of hyaline droplets and minimal to mild eosinophilia of hepatocytes at all dose levels (100, 500, and 1000 mg/kg/day) Significant findings: **1000 mg/kg/day** -Absolute liver and kidney weights were statistically increased in males and females. Liver weights relative to body weight values were statistically elevated in males and females and kidney weights relative to body weights were statistically higher in males only. -In males and females, increased incidences of minimal to mild eosinophilia of hepatocytes and minimal hypertrophy of thyroid follicular epithelium -In males, increased incidence of hyaline droplets in tubular epithelial cells. **500 mg/kg/day** -Absolute liver weights were statistically increased in males and females. Absolute kidney weights were statistically elevated in males -Liver weights relative to body weights were statistically elevated in males and females and kidney weights relative to body weights were statistically higher in males. -In males and females, increased incidences of minimal to mild eosinophilia of hepatocytes and minimal hypertrophy of thyroid follicular epithelium

	-In males, an increased incidence of hyaline droplets in tubular epithelial cells. **100 mg/kg/day** -In males, minimal to mild eosinophilia of hepatocytes and minimal hypertrophy of thyroid follicular epithelium -In males, increased incidence of hyaline droplets in tubular epithelial cells.
Reproductive and Developmental Toxicity	<u>Reproductive and developmental screen (OECD 421) – Oral gavage and rats</u> Reproductive NOEC = 600 mg/kg/day (highest dose) Significant findings: Administration of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide did not adversely impact fertility/reproduction in rats after administration of any dose (50, 175, or 600 mg/kg/day) Litter sizes, fertility indices, pup weights and pup survival were similar between controls and all dose groups. Additionally, administration of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide did not cause any developmental toxicity effects at any dose

7.0 GENETIC TOXICOLOGY DATA

7.1 Mutagenicity

An adequate and reliable bacterial reverse mutation study was performed for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. The material was not mutagenic in any strain in the presence or absence of metabolic activation.

7.2 Clastogenicity

A chromosomal aberration study (OECD 473) was conducted in human peripheral blood lymphocytes. Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide exposure did not result in an increased rate of chromosomal aberrations or endoreduplication in the presence or absence of metabolic activation.

TABLE 5. SUMMARY OF DATA FOR THIOPHENE, 3-(DECYLOXY)TETRAHYDRO-, 1,1-DIOXIDE

CAS Number	Environmental Fate					Ecotoxicity		
	Physical Chem	Photodeg	Hydrolysis	Fugacity	Biodeg	Acute Fish Toxicity	Acute Invert Toxicity	Algal Toxicity
18760-44-6 or 398141-87-2	A/C	C	D	C	A	A	A	A

CAS Number	Human Health Effects				
	Acute Toxicity	Point Mutations	Chrom Effects	Sub-chronic	Repro/ Develop
18760-44-6 or 398141-87-2	A	A	A	A	A

A Adequate data available
C Computer modeling completed
D Technical discussion completed